Perfluorododecanoic acid
307-55-1 | DTXSID8031861

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 244 °C

Global applicability domain: Outside

Local applicability domain index: 1.88e-01

Confidence level: 6.18e-01

Nearest Neighbors from the Training Set

Image not found
Perfluorododecanoic acid
Measured: 249
Predicted: 244

Image not found
PFOA
Measured: 189
Predicted: 188

Image not found
Perfluoroheptanoic acid
Measured: 177
Predicted: 176

Image not found
Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-
Measured: 192
Predicted: 186

Image not found
Sulfluramid
Measured: 196
Predicted: 198